Soliton Fermi Sea in Models of Ising-coupled Kondo impurities

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We study a model of Ising-coupled Kondo impurities that can be applied to quantum dots with capacitance coupling, coupled qubits with an incoherent environment, etc. We show that this model becomes equivalent to a Anderson impurity model with a novel *solitonic Fermi sea*. We derive exact results at the Toulouse point, and use the flow equation method to extend this analysis away from the Toulouse point for not too large Ising couplings.

Introduction. Kondo physics plays a fundamental role for the low-temperature behavior of a large variety of physical systems like magnetic impurities in metals, heavy-fermion systems, glasses, quantum dots, etc. Its key feature is the quenching of the impurity entropy through nonperturbative screening by many-particle excitations in the associated quantum bath. For magnetic impurities in metals this amounts to the formation of the Kondo singlet between the localized spin and electron–hole excitations in the Fermi sea[1].

Most of the aspects of single-impurity Kondo physics are now well understood after theoretical tools have been developed that can deal with its intrinsic strong-coupling nature[2,3]. However, in many physical systems the interaction of different impurities, i.e., multi-impurity Kondo physics, is important. For example in heavy-fermion systems the RKKY interaction between different impurity spins is responsible for the competition between local Kondo physics and long-range magnetic order that determines their phase diagram[4], or in glasses the phonon-mediated coupling between different tunneling centers is known to be important[5]. More recently, related questions about coupled two-level systems have gained much interest in quantum computation, where decoherence due to unwanted couplings among qubits and between qubits and environment should be avoided; on the other hand the intentional coupling of qubits is the key step to performing quantum logic operations.

In the present paper we investigate the case of two Kondo impurities coupled via an S_z-S_z interaction, i.e., an Ising-type coupling. Equivalently, one can think of two two-level systems with transversal coupling, with the experimental realization of coupled flux qubits[6]. Based on the flow equation method[8] we can derive analytical results for this problem by mapping it to a conventional Anderson impurity model. This mapping allows us to derive exact results at the Toulouse point, and controlled approximations in its vicinity. Also we will show how our results can be extended to an arbitrary number of Ising-coupled impurities with an infinite-range interaction.

Coupled impurities or two-level systems have been investigated in a number of papers[9,10,11,12,13], however, most attention has been focussed on the case of SU(2)-symmetric coupling between the impurity spins. We will show that new phenomena arise in the Ising-coupled case due to the two-fold degeneracy of the ground state of the isolated impurity system[14]. In the context of Kondo impurities, this Ising-like coupling can be thought of as an effective impurity interaction for heavy-fermion systems with an easy axis. Also, Ising coupling appears naturally in quantum dots that are coupled via their mutual capacitance: here the two-level systems are pseudospins representing the number of electrons on the dots, and therefore SU(2) symmetry is broken from the outset[15,16,17].

Model. Let us first formulate the model in the language of Kondo impurities. For simplicity, we will consider a situation where the two impurities are placed in different fermionic baths, yielding the Hamiltonian $H^{\rm K} = H_1^{\rm K} + H_2^{\rm K} + H_{12}^{\rm Ising}$, where $H_i^{\rm K}$ are the individual Kondo Hamiltonians

$$H_i^{\rm K} = \sum_{k\alpha} \epsilon_k\, c^\dagger_{k\alpha i} c_{k\alpha i} + J\, \vec{S}_i \sum_{\alpha\beta} c^\dagger_{0\alpha i}\, \vec{\sigma}_{\alpha\beta}\, c_{0\beta i} \qquad (1)$$

with the fermion creation/annihilation operators $c^\dagger_{k\alpha i}$, $c_{k\alpha i}$ with wave vector $k = 2\pi n/L$, $n \in \mathbb{Z}$, spin index α and belonging to Fermi sea $\#i$. $c^\dagger_{0\alpha i}$, $c_{0\alpha i}$ denote the localized electron state at the impurity sites and $\vec{S}_1$, $\vec{S}_2$ are the two spin-1/2 impurities. We will assume a linear dispersion $\epsilon_k = v\,k$ throughout this paper and set $\epsilon_F = 0$. The Ising coupling, which breaks SU(2) symmetry, takes the form

$$H_{12}^{\rm Ising} = K\, S_1^z\, S_2^z\ . \qquad (2)$$

Note that $H_{12}^{\rm Ising}$ has a doubly degenerate ground state for both signs of K. The simplifying assumption of two disconnected baths is naturally satisfied for coupled quantum dots; for magnetic impurities in metals it misses the RKKY interaction, which we instead explicitly include by H_{12}.

The case of SU(2)-symmetric inter-impurity coupling, $K\, \vec{S}_1 \cdot \vec{S}_2$, has been the subject of numerous investigations in the past[9,10,11,12,13]. Generically, two different regimes are possible as function of the inter-impurity exchange K: for large antiferromagnetic K the impurities combine to a singlet, and the interaction with the conduction band is weak, whereas for ferromagnetic K the impurity spins add up and are Kondo-screened by conduction electrons in the low-temperature limit. In both parameter regimes the ground-state spin will be zero,

and there is *no* quantum phase transition as K is varied in the generic situation without particle–hole symmetry (whereas one finds an unstable non-Fermi liquid fixed point in the particle–hole symmetric case)[10,11,12]. However, the finite-T crossover behavior is significantly different in the two regimes: for large antiferromagnetic K, the singlet is formed at an energy scale of order K. In contrast, for ferromagnetic K, where both spins have to be quenched, a two-stage Kondo effect[9,13] occurs if the two screening channels have different Kondo coupling leading to different Kondo temperatures: upon lowering the temperature the two spin-1/2 degrees of freedom are "frozen" at two distinct temperature scales.

An alternative starting point for our model of Ising-coupled impurities can be formulated in terms of two two-level systems (spin–boson models), $H^{\rm SB} = H_1^{\rm SB} + H_2^{\rm SB} + H_{12}^{\rm trans}$ with

$$H_i^{\rm SB} = \frac{\Delta_i}{2}\,\sigma_i^x + \frac{1}{2}\,h_i\,\sigma_i^z + \frac{1}{2}\sum_{k>0}\lambda_{ki}\,\sigma_i^z(b_{ki} + b_{ki}^\dagger) + \sum_{k>0}\omega_{ki}\,b_{ki}^\dagger b_{ki} \qquad (3)$$

and transversal coupling between them, $H_{12}^{\rm trans} = \frac{K}{4}\;\sigma_1^z\,\sigma_2^z$. Here $b_{ki}^\dagger$, b_{ki} are the bosonic creation/annihilation operators for heat bath $\#i$. Δ_i is the bare tunneling matrix element for the two-level system described by σ_x^i, and h_i is the asymmetry of its two wells. The impurity properties are completely parametrized by the spectral function $J_i(\omega) \stackrel{\rm def}{=} \sum_k \lambda_{ki}^2\,\delta(\omega - \omega_{ki})$, which we assume to be of Ohmic form, $J_i(\omega) = 2\alpha_i\,\omega\,e^{-\omega/2\omega_c}$. One realization of this model is the interaction of tunneling centers in glasses through higher-order phonon exchange[5]. In the context of quantum computation this model arises in studies of decoherence of coupled solid state qubits: the transversal coupling K is generated through a superconducting flux transporter, and the heat baths describe the environment leading to decoherence[6,7].

With a polaron transformation $H^{\rm SB}$ can be mapped onto the following Hamiltonian with the same impurity properties, $H^{\rm bos} = H_1^{\rm bos} + H_2^{\rm bos} + H_{12}^{\rm trans}$. Here

$$H_i^{\rm bos} = \frac{1}{2}\,h_i\,\sigma_i^z + g_i\left(V_i(\lambda_i;0)\,\sigma_i^- + {\rm h.c.}\right) + \sum_{k>0} vk\,b_{ki}^\dagger b_{ki} \qquad (4)$$

with coupling constants $g_i = \Delta_i/\sqrt{8}$ and $\omega_{ki} = vk$ without loss of generality. $V_i(\lambda;x)$ denote vertex operators

$$V_i(\lambda;x) \stackrel{\rm def}{=} \exp\Big[\lambda\sum_{k>0}\frac{1}{\sqrt{k}}\,e^{-ak/2}\big(e^{-ikx}b_{ki}^\dagger - e^{ikx}b_{ki}\big)\Big]$$

with scaling dimension $\lambda_i = \sqrt{2\alpha_i}$ and $a = v/\omega_c$.

Eq. (4) is also the bosonized form describing the low-energy properties of the Kondo Hamiltonian (1) with $b_{ki}^\dagger$, b_{ki} describing the spin-density excitations in Fermi sea $\#i$, $a = \rho_F v$, $\lambda_i = \sqrt{2} - (\rho_F J)/\sqrt{8\pi^2}$, $h_i = 0$, and $g_i = J/2$. In the sequel we will use (4) as the unified starting point of our analysis and use the terminology of Kondo impurity problems. Notice that $H_{12}^{\rm trans}$ remained unaffected by the above unitary transformation.

Toulouse point. In a first step to study the phase diagram of Ising-coupled Kondo impurities we investigate the special Toulouse point[18] $\lambda_i = 1$ ($\alpha_i = 1/2$), where we will show that the problem can be solved exactly. Since the vertex operators $V_i(\pm 1;x)$ obey fermionic anti-commutation relations, the Hamiltonian of an individual Kondo impurity, $H_i^{\rm bos}$, can be refermionized, leading to a resonant level model of spinless fermions for each of the two impurities[19]. The Ising coupling transforms into a density–density interaction, and the full model $H^{\rm bos}$ thus reads

$$\begin{aligned} H \;=\; & \sum_{ki} v\,k\,e_{ki}^\dagger e_{ki} + \sum_{ki} V_{ki}\,(e_{ki}^\dagger d_i + d_i^\dagger e_{ki}) \\ & + \epsilon_d(n_{d1} + n_{d2} - 1) + \frac{h_{\rm loc}}{2}\,(n_{d1} - n_{d2}) \\ & + K\left(n_{d1} - \frac{1}{2}\right)\left(n_{d2} - \frac{1}{2}\right) \end{aligned} \qquad (5)$$

with the representation $\sigma_i^+ = d_i^\dagger$, $\sigma_i^- = d_i$, $\sigma_i^z = 2(d_i^\dagger d_i - 1/2)$, $n_{di} = d_i^\dagger d_i$, $V_{ki} = g_i\sqrt{2\pi a/L}$, $\epsilon_d = (h_1 + h_2)/2$, $h_{\rm loc} = h_1 - h_2$, and

$$e_{ki}^\dagger \stackrel{\rm def}{=} \frac{1}{\sqrt{2\pi a L}}\int dx\,e^{ikx}\,V_i(1;x)\ . \qquad (6)$$

Eq. (5) represents one of the main results of our paper: At the Toulouse point the problem of two Ising-coupled Kondo impurities maps onto an *Anderson impurity model* (AIM) with Coulomb interaction K. The Fermi sea of this effective AIM consists of the *soliton excitations* (6) constructed from spin-density excitations around the impurities. The index $i = 1,2$, originally labelling the two impurities and their baths, now plays the role of a pseudospin in this effective AIM. The impurity properties are completely described by the hybridization function $\Delta_i(\epsilon) \stackrel{\rm def}{=} \sum_k V_{ki}^2\,\delta(\epsilon - \epsilon_k)$, which is constant in the above model $\Delta_i(\epsilon) = \rho_F g_i^2$. With this mapping the original problem (at the Toulouse point) is essentially solved since (5) is well-understood using various methods like, e.g., Wilson's numerical renormalization group[2], and for the special case of both impurity sites being equal ($V_{ki} = V$ and $h_{\rm loc} = 0$) is even integrable with exact Bethe ansatz results[3].

This integrable case allows us to study in detail the competition between local Kondo screening and the Ising interaction. From the Bethe ansatz solution one knows that the ground state of the Anderson impurity model is always unique with no phase transition as a function of K. For simplicity we will first analyze the problem with no local magnetic fields $h_1 = h_2 = 0$ ($\epsilon_d = 0$). For large positive $K \gg \Delta(0)$ (large antiferromagnetic Ising interaction) one finds $\langle n_{d1} + n_{d2}\rangle \to 1$ ($\langle S_1^z + S_2^z\rangle \to 0$): the impurity site of the effective Anderson model is singly

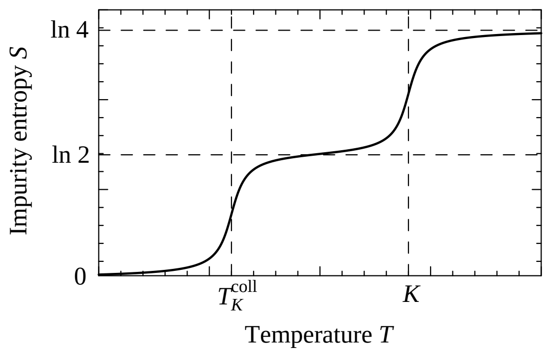

FIG. 1: Schematic temperature dependence of the total impurity entropy of two Ising-coupled Kondo impurities for the case of large inter-impurity coupling, $K \gg T_K^i$. Below K, the impurity spins combine into the two possible (anti)parallel low-energy states for (anti)ferromagnetic K. The remaining pseudospin degree of freedom is screened below $T_K^{\rm coll}$.

occupied. There are two degenerate impurity configurations, namely $\uparrow\downarrow$ and $\downarrow\uparrow$. However, these two configurations get mixed by many-particle excitations in the effective Fermi sea. Thus, the pseudospin is screened below a new *collective Kondo scale* $T_K^{\rm coll} \sim \exp(-|K|/8\Delta(0))$, and the ground state is a singlet. On reducing the temperature the impurity entropy is quenched in two stages (Fig. 1): for $T \gg K$ one finds $S_{\rm imp} = \ln 4$, which is reduced to the two singlet configurations ($S_{\rm imp} = \ln 2$) for temperatures of order K, and finally quenched completely below the collective Kondo temperature $T_K^{\rm coll}$. Note that this type of two-stage screening is completely different from the one mentioned in the introduction[9], which occurs if the two conventional Kondo screening channels have different strengths.

For large negative K (large ferromagnetic Ising interaction) the situation is related to the antiferromagnetic case by particle–hole symmetry: one finds $|\langle S_1^z + S_2^z\rangle| \to 1$, i.e., the two impurity states being degenerate in the absence of the baths are $\uparrow\uparrow$ and $\downarrow\downarrow$. The screening of the associated pseudospin appears at the same collective Kondo scale as above.

For smaller $|K|$, namely of order $\Delta(0)$ or below, the only relevant temperature scale is set by $\Delta(0)$: the two impurities do not couple into an inter-impurity doublet since they are screened individually by their respective Kondo interaction (1) at temperatures above K. Notice that at the Toulouse point $\Delta(0)$ can be identified with the Kondo temperature T_K^i of the individual impurity i, below which screening occurs.

Going away from the integrable case the effective Anderson impurity model (5) still displays the same crossover behavior between the various limiting cases as a function of K, provided that K fulfills Eq. (10) below. In general the above crossover temperatures then depend on ϵ_d and the local magnetic field $h_{\rm loc}$.

Flow equation solution. Next we generalize the exact results at the Toulouse point to general couplings using the flow equation diagonalization of the Kondo Hamiltonian[20]. In Ref. 20 a continuous sequence of unitary transformations was constructed that led to a systematic approximation scheme which becomes exact at the Toulouse point and yields a controlled approximation away from it. This means we know a unitary transformation U_i that diagonalizes the Hamiltonian (4) up to higher-order terms that do not affect the universal properties. It was shown that $\tilde H_i^{\rm bos} = U_i\, H_i^{\rm bos}\, U_i^\dagger$ takes the form

$$\begin{aligned} \tilde H_i^{\rm bos} &= \sum_{k>0} v\,k\, b_{ki}^\dagger b_{ki} + \frac{h_i}{2}\,\tilde\sigma_i^z \\ &\quad + \sum_k \omega_k \left[V(\lambda_i(k);k), V(-\lambda_i(k);k)\right] , \end{aligned} \tag{7}$$

where the third term consists of Fourier transformed vertex operators with a scaling dimension $\lambda_i(k)$ that depends on the energy scale. The unitarily transformed operator $\tilde\sigma_i^z = U_i\, \sigma_i^z U_i^\dagger$ is given by[20]

$$\tilde\sigma_i^z = \sum_{k,k'} \alpha_k \alpha_{k'} \left[V(\lambda_i(k);k), V(-\lambda_i(k');k')\right] \tag{8}$$

with certain coefficients α_k. We now make use of this single-impurity flow equation diagonalization by applying the *combined* unitary transformation $U = U_1\, U_2$ on the coupled system

$$\begin{aligned} \tilde H &= U_1 U_2\, H\, U_2^\dagger U_1^\dagger \\ &= \tilde H_1^{\rm bos} + \tilde H_2^{\rm bos} + \frac{K}{4}\,\tilde\sigma_1^z \tilde\sigma_2^z . \end{aligned} \tag{9}$$

This procedure is summarized in Fig. 2. In the sequel we will only be interested in the strong-coupling regime of the single-impurity problems $\lambda_i^2 \lesssim 2$ implying a flow to the Toulouse point in the infrared limit $\lambda_i(k) \xrightarrow{k\to 0} 1$. We now approximate (8) by setting $\lambda_i(k) = 1 \;\; \forall k$, i.e. by using fermions instead of the vertex operators with a running scaling dimension. This approximation becomes exact in the low-energy limit, where many-particle pseudospin excitations are most important.

Using this approximation (8) can be refermionized leading to a Hamiltonian that has the same structure (5) like at the Toulouse point, except with a non-constant hybridization function $\Delta_i(\epsilon)$ that depends on the unitary transformation U_i. One can show $\Delta_i(0) \sim T_K^i$, and $\Delta_i(\epsilon) \sim \rho_F g_i^2 |\rho_F \epsilon|^{\lambda_i^2 - 1}$ for $|\epsilon| \gg T_K^i$, with a smooth crossover in between[21]. Here T_K^i is the individual Kondo scale of one impurity without Ising coupling to the other impurity.

The above analysis neglects the feedback of one impurity on the other. The accuracy of the approximation within the flow equation transformation U_i decreases away from the Toulouse point. Therefore the error in the transformation of $\tilde\sigma_i^z$ is proportional to the distance to the Toulouse point $(\lambda - 1)$, leading to an error in the transformation of the interaction between the two Kondo impurities that is proportional to $|K\,(\lambda-1)|$. When this

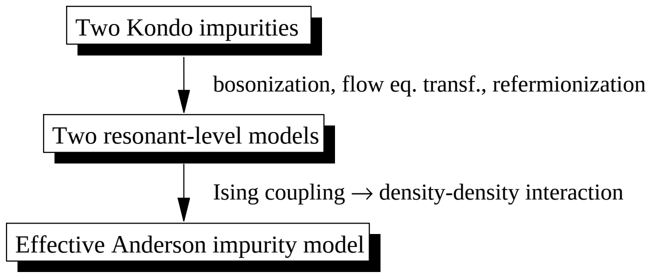

FIG. 2: Steps of our approximate solution of the two-impurity Kondo problem with Ising coupling. Each individual Kondo problem is transformed into an effective spinless resonant-level model by means of a flow-equation transformation. The original Ising coupling maps onto a density–density interaction, leading finally to an Anderson impurity model.

energy scale becomes comparable to the energy scale of the individual Kondo Hamiltonians our approximations are no longer reliable, which means that we can only study the phase diagram for Ising couplings with

$$|K| \ll \frac{\min_i T_K^i}{|\lambda - 1|} \ . \tag{10}$$

For not too large Ising couplings K that fulfill this condition we can trust the mapping to the Anderson impurity model with Coulomb interaction $U = K$, and carry over our analysis from the Toulouse point.

For larger couplings K the flow equation transformation needs to be extended to higher orders. A careful analysis shows that a quantum phase transition can occur when the condition (10) is violated[24]. The Anderson model becomes supplemented by a density–density interaction between the impurity orbital and the first conduction electron site. This interaction maps onto a ferromagnetic spin–spin interaction when charge fluctuations are frozen out for large K; this ferromagnetic interaction can in turn destroy the screening of the pseudospin and lead to a phase with a doubly degenerate ground state. For a full account of this analysis and other approaches to the model of Ising-coupled Kondo impurities we refer to Ref. 23.

N impurities. The above mappings can be generalized to the case of N impurities with infinite-range Ising interaction

$$H = \sum_{i=1}^{N} H_i^K + K \sum_{i<j} S_i^z S_j^z \ . \tag{11}$$

For simplicity we will only look at the Toulouse point (also $h_i = 0 \quad \forall i$), though the above flow equation analysis of the Kondo regime can be carried over as well. After refermionization one finds an N-channel Anderson impurity model describing the SU(N) pseudospin fluctuations:

$$\begin{aligned} H \ =& \ \sum_{ki} v\, k\, e_{ki}^\dagger e_{ki} + \sum_{ki} V_{ki}\, (e_{ki}^\dagger d_i + d_i^\dagger e_{ki}) \\ & + K \sum_{i<j} \left(n_{di} - \frac{1}{2}\right) \left(n_{dj} - \frac{1}{2}\right) \ . \end{aligned} \tag{12}$$

Again the crossover between ferromagnetic and antiferromagnetic coupling K is known to be smooth. For the special case of large positive K – this situation corresponds to a fully frustrated Ising model coupled to dissipative baths – one can perform a generalized Schrieffer–Wolff transformation to an SU(N) Kondo model that describes the quenching of the pseudospin fluctuations below a collective Kondo scale $T_K^{\rm coll}$. Away from the Toulouse point we find the same picture as long as the condition (10) is fulfilled.

Conclusions. Summing up, we have investigated the case of Ising-coupled Kondo impurities. At the Toulouse point we could map this model *exactly* to an Anderson impurity model with a Fermi sea that consists of fermionic soliton excitations. The Ising coupling leads to two degenerate ground states of the isolated double-impurity system; this pseudospin degree of freedom is screened below a collective Kondo scale $T_K^{\rm coll}$ through soliton excitations. This piece of physics describing many-particle excitations of solitons (*many-many-particle excitations*) is absent for an SU(2)-symmetric inter-impurity coupling. Using the novel flow equation method[8,20] we could extend this analysis from the Toulouse point for not too large Ising couplings K that obey Eq. (10).

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[24] A previous version of this preprint did not take into account the effects that are due to the flow equation approximations away from the Toulouse point and incorrectly concluded that there is no phase transition for all values of K even away from the Toulouse line.